

Contribute to BRENDA! Your enzyme data is important for BRENDA. Send us your paper, and we will do all the work to include your data into our database. [More...](#)

Please enter a search term

Enzyme, Ligand contains

add search field delete search field **start search**

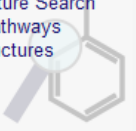
Text-based queries

- Full-text Search
- Advanced Search
- Enzyme & Disease



Structure-based queries

- Ligand Structure Search
- Metabolic Pathways
- Enzyme Structures



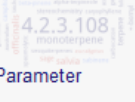
Explorer

- Enzyme Classification
- TaxTree
- Protein folding: CATH / SCOPe
- Ontologies



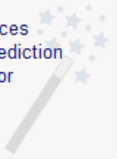
Visualization

- Word Maps
- Genomes
- Functional Parameter Statistics
- Metabolic Pathways



Prediction

- Membrane Helices
- Localization Prediction
- EnzymeDetector



Supporting & External


- BRENDA Tissue Ontology
- Biochemical Reactions
- MetaboMAPS



News

NEW Release online! - February 1, 2021
Release 2021.1 online including 76 new and 623 updated enzyme classes.

for Release 2021.1



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Information

BRENDA Tutorial

Ligand Search

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Please enter a search term

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add search field delete search field **start search**

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for Release 2021.1

How to find ligands / metabolites such as substrates, products, inhibitors etc. Substances interacting with enzymes

Contribute to BRENDA! Your enzyme data is important for BRENDA. Send us your paper, and we will do all the work to include your data into our database. More...

vanillic acid

Enzyme, Ligand contains

add search field delete search field start search

Text-based queries

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Structure-based queries

- Ligand Structure Search
- Metabolic Pathways
- Enzyme Structures

Explorer

- Enzyme Classification
- TaxTree
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- Ontologies

Visualization

- Word Maps 4,23,108
- Genomes
- Functional Parameter Statistics
- Metabolic Pathways

Prediction

- Membrane Helices
- Localization Prediction
- EnzymeDetector

Supporting & External

- BRENDA Tissue Ontology
- Biochemical Reactions
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Enter the ligand name or a part of it and perform the search

News

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Refine search

Field	Hits found
Enzyme Names (Synonyms)	1
Ligands	43

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UPDATE!



Choose „Ligands“ to display the enzyme-related information on vanillic acid








































































Search Ligands



Search term: vanillic acid

Refine search


The result page shows all enzymes interacting with the ligand, including their derivatives, and their roles


« « Results 1 - 10 of 43 » »
 download as CSV
 download all results as CSV

Ligand ▼▲	EC Number ▼▲	Role ▼▲	Structure ▼▲
vanillic acid	   1.1.1.21	Inhibitor	    
vanillic acid	  1.1.99.20	Product	    
vanillic acid	  1.10.3.2	KM Value, Substrate, Turnover Number	    
vanillic acid	  1.11.1.1	Activating Compound	    
vanillic acid	  1.11.1.7	KM Value, Substrate	    
vanillic acid	  1.13.11.3	Substrate	    
vanillic acid	  1.14.13.82	Natural_Product, Natural_Substrate, Product, Substrate	    
vanillic acid	  1.14.18.1	Substrate	    
vanillic acid	  1.2.1.3	Product	    
vanillic acid	  1.2.1.30	Substrate	    

« « Results 1 - 10 of 43 » »
 download as CSV
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BRENDA - Chemical structure of vanillic acid - Mozilla Firefox

www.brenda-enzymes.org/structure.php?n=1882

BRENDA

vanillic acid = Search

Search again for: [vanillic](#), [acid](#)

Chemical structure of vanillic acid

COc1ccc(cc1C(=O)O)O

BRENDA The Comprehensive Enzyme Information System

Technische Universität Braunschweig

Contact

login history all enzymes

Refine search

you can display the molecular structure

Role	Structure
1.21 Inhibitor	
.20 Product	
.2 KM Value, Substrate, Turnover Number	
.1.1 Activating Compound	
.1.7 KM Value, Substrate	
.11.3 Substrate	
3.82 Natural_Product, Natural_Substrate, Product, Substrate	
8.1 Substrate	
1.3 Product	
Substrate	

« « Results 1 - 10 of 43 » »

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Refine search

Search Ligands

Search term: vanillic acid

On the next page you get basic information on the Ligand Summary Page with...



Ligand	EC Number		
vanillic acid			
vanillic acid	1.1.99.20	Product	
vanillic acid	1.10.3.2	KM Value, Substrate, Turnover Number	
vanillic acid	1.11.1.1	Activating Compound	
vanillic acid	1.11.1.7	KM Value, Substrate	
vanillic acid	1.13.11.3	Substrate	
vanillic acid	1.14.13.82	Natural_Product, Natural_Substrate, Product, Substrate	
vanillic acid	1.14.18.1	Substrate	
vanillic acid	1.2.1.3	Product	
vanillic acid	1.2.1.30	Substrate	

Results 1 - 10 of 43
download as CSV
download all results as CSV

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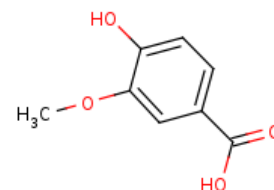


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Ligand vanillic acid

Basic Ligand Information

Molecular Structure



...more detailed information on the structure, synonyms, and their roles in the enzyme-ligand interaction, enzyme kinetic parameters, and references in BRENDA

Molecular Formula	BRENDA Name	InChIKey
C ₈ H ₈ O ₄	vanillic acid	FSQQTNAZHBEJLS-UPHRSURJSA-N

Synonyms:

3-methoxy-4-hydroxybenzoate, 3-methoxy-4-hydroxybenzoic acid, 4-hydroxy-3-methoxy-benzoate, 4-hydroxy-3-methoxybenzoate, 4-hydroxy-3-methoxybenzoic acid, 4-hydroxy-3-methoxy benzoic acid, vanillate, vanillinic acid

Pathway Source	Pathways
KEGG	Aminobenzoate degradation , Microbial metabolism in diverse environments
MetaCyc	5,5'-dehydrodivanillate degradation , cyanidin diglucoside biosynthesis (acyl-glucose dependent) , delphinidin diglucoside biosynthesis (acyl-glucose dependent) , pelargonidin diglucoside biosynthesis (acyl-glucose dependent) , pinoresinol degradation more

[✖ close all tables](#) [✚ open all tables](#)

Roles as Enzyme Ligand

In Vivo Substrate in Enzyme-catalyzed Reactions (7 results)

[△ top](#) [print](#) [hide](#) [☒](#)

EC NUMBER ▲▼	PROVEN IN VIVO REACTION ▲▼	REACTION DIAGRAM	LITERATURE ▲▼	ENZYME 3D STRUCTURE ▲▼
1.14.13.82	☒ 5 entries			
2.1.1.341	☒ 2 entries			

















Refine search



Search Ligands

Search term: vanillic acid

you can directly switch to the „Substructure Search“ to find similar ligands interacting with enzymes in BRENDA



		Structure ▾
vanillic acid	  1.10.3.2	KM Value, Substrate, Turnover Number
vanillic acid	  1.11.1.1	Activating Compound
vanillic acid	  1.11.1.7	KM Value, Substrate
vanillic acid	  1.13.11.3	Substrate
vanillic acid	  1.14.13.82	Natural_Product, Natural_Substrate, Product, Substrate
vanillic acid	  1.14.18.1	Substrate
vanillic acid	  1.2.1.3	Product
vanillic acid	  1.2.1.30	Substrate

« « Results 1 - 10 of 43 » »
 download as CSV
 download all results as CSV

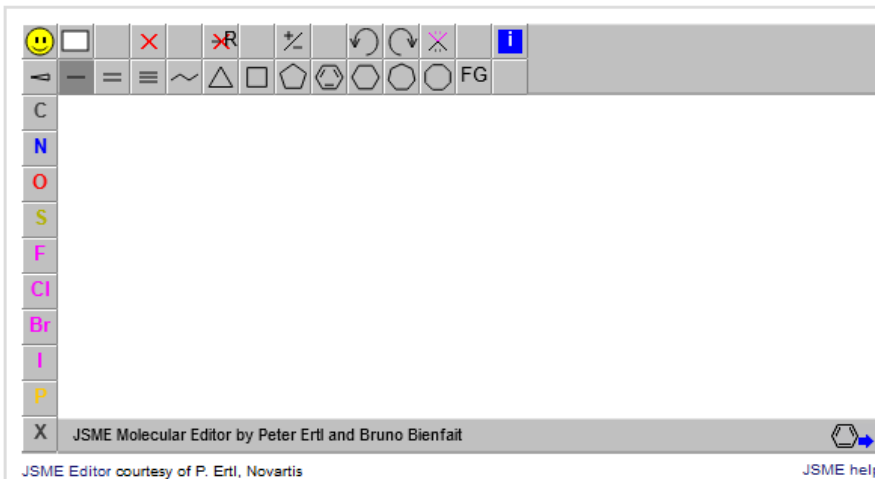
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Structure Search ▢



JSME Molecular Editor by Peter Ertl and Bruno Bienfait

JSME Editor courtesy of P. Ertl, Novartis JSME help

Search Options

Select search type

Select maximal se

Restrict the search

On the result page all ligands structurally similar to the searched ligand are displayed

Search

Molecules containing vanillic acid:

47 entries found in 5 seconds, scanned 110 of 125 fingerprint hits (88%) ▢

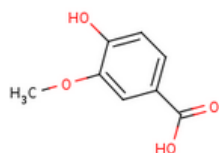
Results 1 to 12 of 47 ▸ ▹

> Filter the results

vanillic acid

Synonyms:

vanillate, 4-hydroxy-3-methoxybenzoate, 4-hydroxy-3-methoxybenzoic acid, 3-methoxy-4-hydroxybenzoate, 4-hydroxy-3-methoxy benzoic acid, 3-methoxy-4-hydroxybenzoic acid, 4-hydroxy-3-methoxy-benzoate, vanillic acid



Roles:

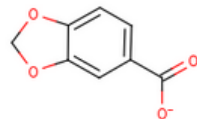
- Substrate
- Product
- Activating Compound
- Inhibitor

[BRENDA search](#)

(3,4-Methylenedioxy)benzoate

Synonyms:

3,4-Methylenedioxybenzoate



Roles:

- Substrate
- Product

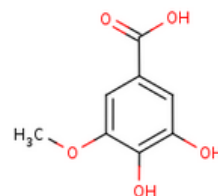
[BRENDA search](#)

[Ligand Summary Page](#)

5-methoxygallic acid

Synonyms:

3-O-methylgallate, 3-Methoxygallic acid, 3,4-dihydroxy-5-methoxybenzoate



Roles:

- Substrate
- Product

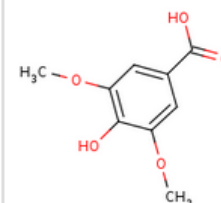
[BRENDA search](#)

[Ligand Summary Page](#)

syringic acid

Synonyms:

syringate, 4-hydroxy-3,5-dimethoxybenzoic acid, 3,5-Dimethoxy-4-hydroxybenzoate, 3,5-Dimethoxy-4-hydroxybenzoic acid, 4-hydroxy-3,5-dimethoxy benzoic acid, 3,5-dimethoxy 4-hydroxybenzoic acid

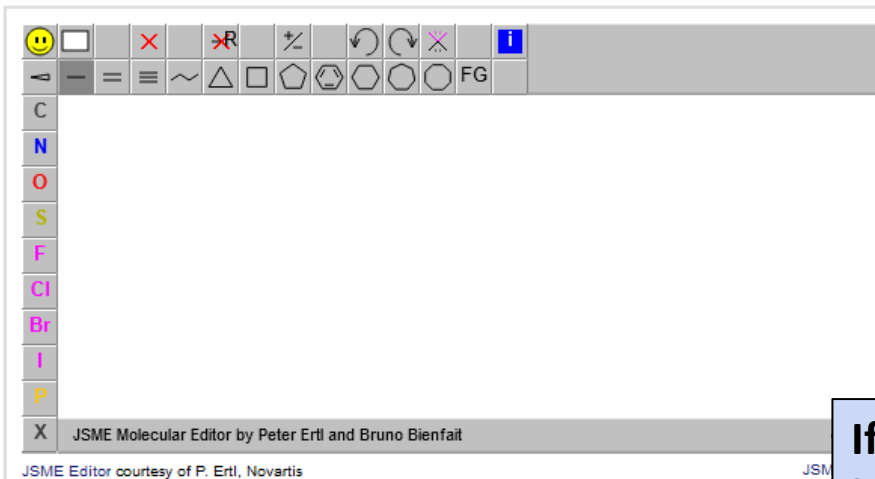


Roles:

- Substrate
- Product
- Activating Compound
- Inhibitor

[BRENDA search](#)

Structure Search ▢



JSME Molecular Editor by Peter Ertl and Bruno Bienfait

JSME Editor courtesy of P. Ertl, Novartis

Search Options

- Select search type:
- Select maximal search time:
- Restrict the search to:
- Substrates
 - Products
 - Cofactors
 - Activating Compounds
 - Inhibitors

If you find an appropriate ligand, you can perform a search in BRENDA to get more information

Molecules containing vanillic acid:

47 entries found in 5 seconds, scanned 110 of 125 fingerprint hits (88%) ▢

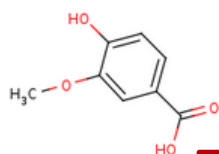
Results 1 to 12 of 47 ▸ ▹

> Filter the results

vanillic acid

Synonyms:

vanillate, 4-hydroxy-3-methoxybenzoate, 4-hydroxy-3-methoxybenzoic acid, 3-methoxy-4-hydroxybenzoate, 4-hydroxy-3-methoxy benzoic acid, 3-methoxy-4-hydroxybenzoic acid, 4-hydroxy-3-methoxy-benzoate, vanillinic acid



Roles:

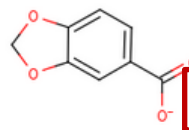
- Substrate
- Product
- Activating Compound
- Inhibitor

[BRENDA search](#)

(3,4-Methylenedioxy)benzoate

Synonyms:

3,4-Methylenedioxybenzoate



Roles:

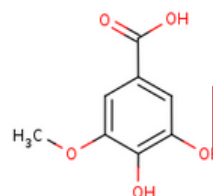
- Substrate
- Product

[BRENDA search](#)
[Ligand Summary Page](#)

5-methoxygallic acid

Synonyms:

3-O-methylgallate, 3-Methoxygallic acid, 3,4-dihydroxy-5-methoxybenzoate



Roles:

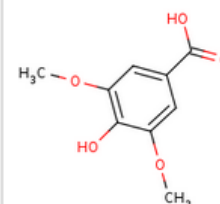
- Substrate
- Product

[BRENDA search](#)
[Ligand Summary Page](#)

syringic acid

Synonyms:

syringate, 4-hydroxy-3,5-dimethoxybenzoic acid, 3,5-Dimethoxy-4-hydroxybenzoate, 4-hydroxy-3,5-dimethoxy benzoic acid, 3,5-dimethoxy 4-hydroxybenzoic acid



Roles:

- Substrate
- Product
- Activating Compound
- Inhibitor

[BRENDA search](#)

Refine search

Search Ligands

Ligands show results

Don't show organism specific information (fast!)

Search organism in taxonomic tree (slow, choose "exact" as search mode, e.g. "mammalia" for rat,human,monkey,...)

(Not possible to combine with the first option)

Refine your search

EC Number: contains

Role: contains

Organism: contains

inchi: contains

Reference: contains



Image of 2D Structure









Search for synonyms (with exact matching search term)



On the result page you find further details of the searched ligand

The synonyms for **(3,4-Methylenedioxy)benzoate** are:
(3,4-Methylenedioxy)benzoate, 3,4-Methylenedioxybenzoate
[Ligand Summary Page](#)

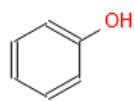
Search term: (3,4-Methylenedioxy)benzoate

« Results 1 - 2 of 2 »
 download as CSV
 download all results as CSV

Source	Ligand ▼▲	EC Number ▼▲	Role ▼▲	Structure ▼▲
BRENDA	(3,4-methylenedioxy)benzoate	 3.5.5.7	Product	  
BRENDA	3,4-methylenedioxybenzoate	 1.14.99.15	Substrate	  

« Results 1 - 2 of 2 »
 download as CSV
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Structure Search ▢



JSME Editor courtesy of P. Ertl, Novartis

Search Options

Select search type:

Substructure Search ▾
 Substructure Search

Select maximal search time:

Similarity
 Isomers

Restrict the search to:

- Substrates
- Products
- Cofactors
- Activating Compounds
- Inhibitors

[Search](#)

Otherwise you could perform a new Substructure Search by drawing the molecular structure with the editor and choosing appropriate search options.

Molecules containing vanillic acid:

47 entries found in 5 seconds, scanned 110 of 125 fingers

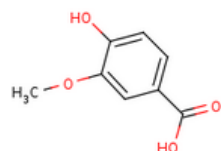
Results 1 to 12 of 47 >>>

> Filter the results

vanillic acid

Synonyms:

vanillate, 4-hydroxy-3-methoxybenzoate, 4-hydroxy-3-methoxybenzoic acid, 3-methoxy-4-hydroxybenzoate, 4-hydroxy-3-methoxy benzoic acid, 3-methoxy-4-hydroxybenzoic acid, 4-hydroxy-3-methoxy-benzoate, vanillinic acid



Roles:

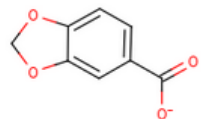
- Substrate
- Product
- Activating Compound
- Inhibitor

[BRENDA search](#)

(3,4-Methylenedioxy)benzoate

Synonyms:

3,4-Methylenedioxybenzoate



Roles:

- Substrate
- Product

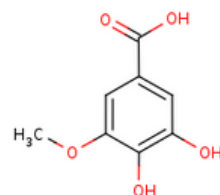
[BRENDA search](#)

[Ligand Summary Page](#)

5-methoxygallic acid

Synonyms:

3-O-methylgallate, 3-Methoxygallic acid, 3,4-dihydroxy-5-methoxybenzoate



Roles:

- Substrate
- Product

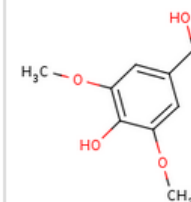
[BRENDA search](#)

[Ligand Summary Page](#)

syringic acid

Synonyms:

syringate, 4-hydroxy-3,5-dimethoxybenzoic acid, 3,5-Dimethoxy-4-hydroxy-benzoate, 3,5-Dimethoxy-4-hydroxybenzoate, 4-hydroxy-3,5-dimethoxy benzoic acid, 3,5-dimethoxy 4-hydroxybenzoic acid



Roles:

- Substrate
- Product
- Activating Compound
- Inhibitor

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